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Modeling phase change materials embedded in building enclosure: A review

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ABSTRACT

Thermal energy storage (TES) has the capability to absorb, store and release heat based on dynamic surrounding environmental conditions. Sensible energy storage captures or releases heat with changes in material's temperature while latent heat is associated with a phase change at an isotherm or near isothermal temperature. Latent heat storage such as using a phase change material (PCM) gains growing attentions recently due to its ability of storing significant thermal energy within a small volume, making it one of most promising technologies for developing energy efficient buildings. To quantify their technical and economic feasibility for building's applications, computational models of TES that can be integrated into whole building energy simulations are highly demanded. This paper reviews the different modeling methods generally used for PCM simulations. A few numerical modeling methods are observed in literature for modeling PCMs including the enthalpy method, the heat capacity method, the temperature transforming model, and the heat source method. The study compares and highlights the advantages, disadvantages and limitations of these models and methods. It particularly explores the viability of these methods for building applications. The paper further reviews the PCM models that have been integrated into prevalent whole building simulation programs such as EnergyPlus, TRNSYS, ESP-r etc. The study reveals that the heat capacity method is mostly used in programs, despite of its limitations on time and spatial resolutions. Further research is found necessary to identify the efficiency and accuracy of these methods in building applications.

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1. Introduction

Thermal energy storage (TES) or thermal mass is a property of materials that describes its ability to absorb, store and release heat depending on the surrounding environmental conditions. Traditional architecture, for example, is distinguished with its heavy weight and thermally massive construction elements to moderate the indoor environment extremes experienced in hot or cold days. The thermal properties of construction elements have significantly improved thermal comfort by manipulating the indoor air temperature without the need of mechanical air conditioning systems [1]. On the other hand, light weight buildings are characterised by its lower thermal mass and thus expose to significant temperature swings, demanding high cooling and heating energy. A dynamic thermal mass such as phase change materials (PCM) has been considered as a promising technology to reduce the inherited climatic deficiency in light weight buildings.

The apparent advantage of using PCMs lies on the amount of latent heat a thin PCM layer can store compared to that in a sensible heat storage material such as concrete. For instance, a wall of 25 mm thickness with PCM could store an equivalent amount of thermal energy as a 420 mm thick concrete wall [2]. As a result, the use of PCMs has recently attracted great attentions for improving thermal and energy performance of buildings [3–8]. Recent studies that review PCMs in building applications can be found in [9–18]. Various challenges are, however, arisen when using PCM in buildings, including the variety of materials available, material liability and safety, cost and economic feasibility, design configurations, integration with other sustainable energy technologies, impact on thermal and energy performance. The problem can then be considered as an optimization dilemma where all these counterparts' challenges are becoming critical in the design process. As a result, computational modeling is often used as an effective tool to quantitatively understand and help resolving this optimization problem.

This review paper adds to the already existing studies that discuss the mathematical modeling of phase change materials for building applications such as those described in [19–21]. The objective of this study is to systematically review the general modeling theories and techniques for PCM, with an emphasis on the specific models used for simulating the thermal and energy performance of PCMs embedded in building enclosures. Furthermore, this paper reviews and summarizes the capabilities, limitations and validations of prevalent whole building simulation programs that have been used for modeling phase change materials.

2. General formulation of phase change problems

The main feature of phase change problems (i.e., Stefan problems) is the moving boundary where the Stefan condition must be met. For pure materials there is a clear distinction between the solid and liquid phase separated by a sharp moving interface and hence melting occurs at isothermal temperature. For conduction-dominated heat transfer, the governing equation can be written for the solid and liquid phase, respectively, which have to be satisfied by the Stefan condition as follows [22]:

Heat transfer in the solid phase:

$$\rho \times c_s \times \frac{\partial T_s}{\partial t} = \frac{\partial}{\partial x}\left(k_s \times \frac{\partial T_s}{\partial x}\right) \tag{1}$$

Heat transfer in the liquid phase:

$$\rho \times c_l \times \frac{\partial T_l}{\partial t} = \frac{\partial}{\partial x}\left(k_l \times \frac{\partial T_l}{\partial x}\right) \tag{2}$$

The Stefan condition that enforces the heat balance at the solid–liquid interface is:

$$\frac{\partial}{\partial x}\left(k_s \times \frac{\partial T_s}{\partial x}\right) \times n - \frac{\partial}{\partial x}\left(k_l \times \frac{\partial T_l}{\partial x}\right) \times n = \rho \times L \times v \times n \tag{3}$$

Very few analytical solutions are available in the closed form for phase change problems and can be found in advanced heat transfer books such as those by Crank [23], Alexiades and Solomon [24], and Özıs¸ık [25]. Therefore, approximate numerical solutions are usually used to handle this class of problems. The numerical methods for addressing these problems have been reviewed in literature [26–29] and can be generally divided into:

1. Fixed grid method (i.e., weak solution): These methods consist of fixed space grids where the boundary is tracked by the use of an auxiliary function. Different approaches are employed to account for latent heat evolution [27,29,30]. This class of methods has been widely used and therefore will be the focus of this paper.
2. Deforming grid method or front tracking scheme (i.e., classical solution or strong numerical solution): These methods allow the grid nodes move along with the moving boundary layer and thus the space girds deform as the solution develops. Here the interface is explicitly tracked using the Stefan condition [24].
3. Hybrid method: These methods utilize the features of both fixed and deforming grids which uses a fixed background grid and employs local front tracking schemes to follow the movement of the boundary [26].

3. Numerical formulation of phase change problems using fixed grid methods

An intuitive approach in solving phase change problems is to explicitly follow the moving boundary using the front-tracking

Nomenclature

a	*matrix coefficient*
c	specific heat capacity
f	fluid fraction of PCM
h	enthalpy
k	thermal conductivity
L	latent heat of fusion
n	the unit normal on the phase interface
S	source term
T	temperature
t	time
v	velocity of the interface
x	space distance

Greek letters

$\in$	half range melting temperature
ρ	density

Subscripts and superscripts

A	Apparent
avg	average
e	east node
eff	effective
l	liquid state
m	melting
n	iteration level
p	point node
s	solid state
w	west node

methods. However, this method needs to make a *priori* assumption that the boundary is smooth or monotonic during the period [31]. This assumption is not always true and therefore reformulating phase change problems using the fixed grid techniques becomes an obvious alternative [23,30,32,33]. The Stefan condition Eq.(3) within the fixed grid method is implicitly treated by the reformulated governing equation and hence the position of the moving boundary is known when the solution is converged.

The fixed grid method is simple compared to the others, most versatile, convenient, adaptable and easily-programmable [24]. The latent heat evolution is accounted for in the governing equation by using either enthalpy method [34–38], heat capacity method [39–42], temperature transforming model [43–46], heat source method [38,47–50], or other methods [27,29,51]. The following sections will describe the widely used methods.

3.1. The enthalpy method

In the Enthalpy method, the latent and specific heat are combined into an enthalpy term in the governing equation. The enthalpy method was proposed by Eyres [38] to deal with variations of thermal properties with respect to temperature. For conduction-dominated heat transfer, the governing Eqs. (1)–(3) can be reformulated into one equation where the latent heat is absorbed into the enthalpy term as follows:

$$\rho \frac{\partial h}{\partial t} = \frac{\partial}{\partial x}\left(k\,\frac{\partial T}{\partial x}\right) \tag{4}$$

To demonstrate this method, a fully implicit control volume approximation of Eq. (4) for a typical grid shown in Fig. 1

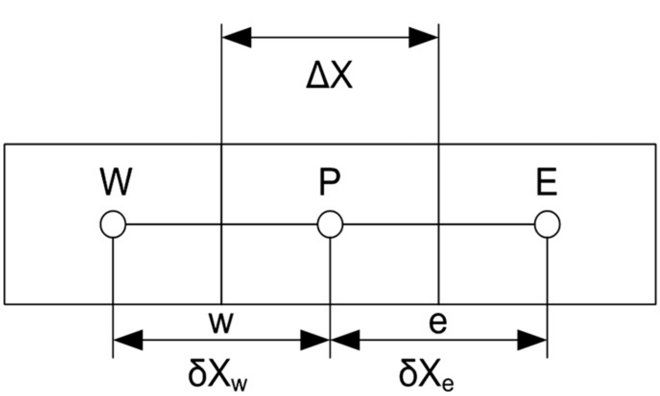

Fig. 1. A typical control volume grid.

leads to the following discretized equation:

$$h_p^{n+1} = h_p^n + a_w^{n+1} \times T_w^{n+1} + a_p^{n+1} \times T_p^{n+1} + a_e^{n+1} \times T_e^{n+1} \tag{5}$$

According to Eq. (5), it is clear that the current enthalpy (h_p^{n+1}) is dependent on the current value of temperature (T_p^{n+1}) and therefore the enthalpy term is nonlinear. The equation cannot be solved without using proper numerical techniques to handle this nonlinearity. This has to be solved either by nonlinear solvers such as the Newton's method or by linearizing the nonlinear terms and utilizing iterative methods as fully explained by [24,30,31,34,35,52–56]. If a non-linear solver is selected, an auxiliary temperature–enthalpy function is required for Eq. (5) and can be written for materials that change phases at specific temperature range as follows [22]:

$$T_p = \begin{cases} \dfrac{h_p}{C_s}, & h_p \le C_s \times (T_m - \in) \\ \dfrac{h_p + \left[\frac{C_l - C_s}{2} + \frac{L}{2\times\in}\right] \times (T_m - \in)}{\left[\frac{C_l - C_s}{2} + \frac{L}{2\times\in}\right]}, & C_l \times (T_m - \in) < h_p < C_s \times (T_m + \in) + L \\ \dfrac{h_p - (C_s - C_l)\times T_m - L}{C_l}, & h_p \ge C_l \times (T_m + \in) + L \end{cases} \tag{6}$$

Alexiades and Solomon [24] have outlined numerical schemes for solving phase change problems with the enthalpy method using both linear and nonlinear approaches. Knoll on the other hand reviewed various approaches utilizing nonlinear solvers to resolve the Stefan problem [55]. He, in particular, developed an algorithm to solve the Stefan problem using the Jacobian-free Newton–Krylove method and applied for two scenarios: (1) pure materials where melting occurs at isothermal temperature and (2) non-isothermal case where phase change occurs at a range of melting temperature.

An alternative approach to solving the discretized Eq. (5) is to linearize the nonlinear term, $h_p^{n+1}(T)$, using the methods explained by Patankar [57]. The discretized nonlinear equation becomes linear with one primary dependent variable "Temperature" that can be iteratively solved with enthalpy using common linear solvers such as direct methods (e.g., Gauss elimination or tri-diagonal algorithm) or iterative methods (e.g., Gauss–Seidel method). Shamsunder [34], for example, proposed a Gauss–Seidel iterative scheme where the solution sweeps from west to east to determine the state of phase change and subsequently determine the new nodal enthalpy. The nodal temperatures are then determined based on the discrete form of the enthalpy–temperature relationship. To avoid excessive iterations, the scheme was later improved by introducing an over-relaxation parameter that is used at nodes where no phase change occurs [58]. The scheme was however intended for phase change that occurs at isothermal

temperature. An iterative Newton linearization scheme was introduced by Furzeland [31]. The solution process is the same as that of Shamsunder except that the over-relaxation parameter can be applied at all nodes.

Iterative methods such as Gauss–Seidel are inherently slow and computationally inefficient. Therefore, fast numerical schemes have been introduced to improve the computational efficiency [35,42,48]. Pham [42] proposed a method that combines the features of the enthalpy and heat capacity methods. The method consists of two steps: a prediction step followed by a correction step as shown in Fig. 2. Based on guessed values, the new nodal temperatures are predicted (point (2) on the graph). The enthalpy is determined based on the predicted temperature values. The predicted temperatures are subsequently corrected to be consistent with the enthalpy–temperature curve (point (3) on the graph). This temperature correction step is the key of this method. This method is later known to be the *"Quasi-Enthalpy"* method [59].

Voller pointed out that this method might not conserve energy at every time step [22] and a better conservative iterative scheme was proposed by Swaminathan and Voller as illustrated in Fig. 3 [35]. The method iterates the predicted and corrected intermediate values until the convergence is achieved. The method has been recently investigated as an alternative to overcome the limitations of the PCM simulation algorithm implemented in ESP-r [60].

3.2. *The heat capacity method*

The heat capacity term in the governing equation imitates the effect of enthalpy (sensible and latent heat) by increasing the heat capacity value during the phase changing stage. Two approaches are generally used to account for the latent heat liberation: the apparent heat capacity [22,27,29] and the effective heat capacity [61,62]. Although the two approaches differ in the heat capacity approximation, recent literatures, however, use the terminologies interchangeably. More details on the effective heat capacity concept are explained by Poirier [63].

The apparent heat capacity method was introduced by Hashemi and Sliepcevich [64] to solve a one-dimensional heat transfer with phase change in a mushy region. The conduction-dominated one-dimensional heat transfer equation using the

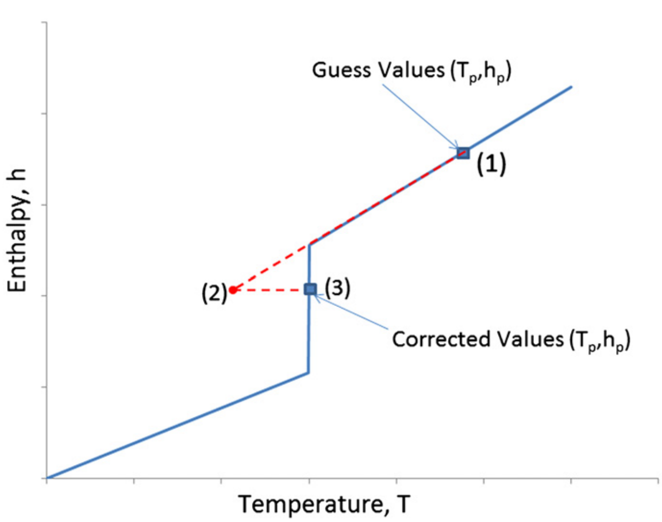

Fig. 2. Corrective non-iterative scheme in the Quasi–Enthalpy method at a node during one time step.

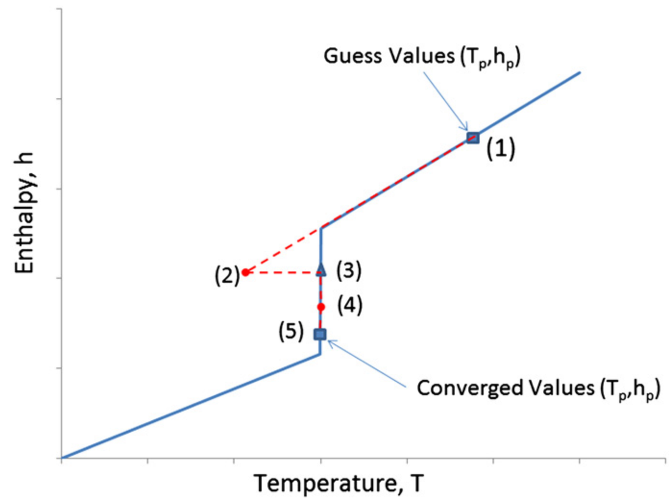

Fig. 3. Corrective iterative scheme in the Enthalpy method at a node during one time step.

apparent heat capacity can be written as:

$$\rho \times C^A(T) \times \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(k\,\frac{\partial T}{\partial x}\right) \quad (7)$$

The method receives the popularity because the temperature is the only prime variable that needs to be solved in the discretized form. The key in this approach lies in the heat capacity approximation. Two methods are commonly used to approximate the apparent heat capacity term in Eq. (7): the analytical/empirical relationships and the numerical approximations.

3.2.1. *The analytical/empirical relationships*

The heat capacity of a PCM can be determined from the testing data with differential scanning calorimeters (DSC). Manufacturers of PCMs normally provide limited data pertained to their products such as melting temperature, heat of fusion and heat capacity at solid and liquid states. Such minimal data can be used to approximate the heat capacity of a PCM using a simple direct relationship with an introduction of fictitious melting temperature range ($2 \times \in$) [22,43]:

$$C^A = \begin{cases} C_s, & T \le T_m - \in \quad \text{(Solid region)} \\ \frac{C_s + C_l}{2} + \frac{L}{2\in}, & T_m - \in \; < T < T_m + \in \quad \text{(Mushy region)} \\ C_l, & T \ge T_m + \in \quad \text{(Liquid region)} \end{cases} \quad (8)$$

Convergence might be an issue when solving Eq. (7), if the half phase change range ($\in$) is set too small or the time step is too large. There is a possible risk of missing the latent heat contribution in a large time step. Hence, DSC testing results can be used to form an empirical expression to approximate the heat capacity. Fang [65], for instance, proposed a mathematical expression for the heat capacity of paraffin—based PCM obtained from DSC. Others have suggested and used alternative forms to approximate the heat capacity [66–69].

3.2.2. *The numerical approximations*

Numerical approximation is an alternative when detailed information about PCM's thermal behaviors is available. Many numerical approximations have been proposed in literature [41,70–75]. For example, Comini [70] applied a numerical technique in the finite element method where the heat capacity was determined using a derivative of enthalpy with respect to temperature. Later, Morgan [71] has improved the relationship to avoid the convergence problems. When using an iterative scheme,

the heat capacity can be approximated using the successive temperature and enthalpy solutions. The temporal averaging proposed by Morgan [71] is illustrated in Fig. 4 and is represented by the following equation:

$$C^A = \frac{\Delta h}{\Delta T} = \frac{h^n - h^{n-1}}{T^n - T^{n-1}} \tag{9}$$

On the other hand, Lemmon [73] proposed an approximation based on the space average rather than the time average approach. The temporal and space average approximations are, however, prone to convergence issues unless some precautions are taken [76]. Solutions to the limitations of the apparent heat capacity method have been proposed in literature [33,61,77–79]. Voller [22] found that the apparent heat capacity approximation based on the direct relationships are more accurate than the Morgan approximation used for the cases he studied.

3.3. The temperature transforming model

The temperature transforming model was developed by Cao and Faghri [80] to overcome the time and spatial limitations in the heat capacity method. The model has been used by Faghri and his co-workers for many applications [44,45,81]. The method is also called "the improved temperature-based equivalent heat capacity method" [82]. While the method was tested against several benchmark examples, it has been reported to produce inconsistent results especially when mass transfer through PCM is considered. Corrections were proposed to improve the accuracy [81,82]. The key of this method is that the energy Eq. (4) is transformed into a nonlinear Eq. (10) with a single dependent variable "Temperature" [43].

$$\rho \times C_{eff}(T) \times \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(k\,\frac{\partial T}{\partial x}\right) - \rho \times \frac{\partial S}{\partial t} \tag{10}$$

This source term is represented by the following Equation [43].

$$S(T) = \begin{cases} C_s \times \in, & T < T_m - \in \\ \left(\frac{C_s + C_l}{2}\right) \times \in \; + \; \frac{L}{2}, & T_m - \in \; < T < T_m + \in \\ C_l \times \in \; + \; L, & T > T_m + \in \end{cases} \tag{11}$$

The latent heat during the phase change stage is represented by a source term in the governing equation with the heat capacity term similar to the apparent heat capacity method. The method is, however, not commonly used but offers an alternative solution when compared to the apparent heat capacity method.

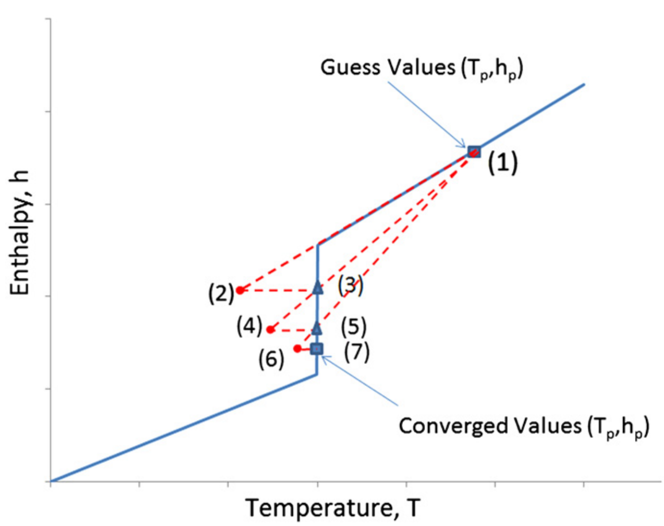

Fig. 4. Apparent heat capacity approximation at a node during one time step using iterative methods.

3.4. The heat source method

Using the heat source method, the total enthalpy in the governing Eq. (4) is split into the specific heat and latent heat where the latent heat acts as a source term [23,47]. Eq. (4) thus becomes:

$$\rho \times C_{avg} \times \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(k\,\frac{\partial T}{\partial x}\right) - \rho \times L \times \frac{\partial f_l}{\partial t} \tag{12}$$

The method was alluded by Eyres [38] in the mid-1940s. In popular schemes, the phase change front is tracked by the evaluation of a nodal liquid fraction field which takes a value of 0 for solid, 1 for liquid, and a value in the range of [0–1] for the mushy region [23,49]. With this approach, the fluid fraction is linearized and the equation can be solved iteratively with temperature. The liquid fraction can be approximated using the following auxiliary equation [49]:

$$f_l = \begin{cases} 0, & \text{if } T \le T_m - \in \\ \frac{(T - T_s)}{(T_L - T_s)}, & \text{if } T_m - \in \; < T < T_m + \in \\ 1, & \text{if } T \ge T_m + \in \end{cases} \tag{13}$$

When discretizing Eq. (12) with a fully implicit scheme and linearizing the source term "liquid fraction" at the current time step, the discretized equation becomes linear and needs to be solved for temperature in an iterative manner with the liquid fraction. Costa [50] has used this method to numerically simulate the latent heat thermal storage.

3.5. Summary

Different mathematical models and methods have been suggested in literature to deal with phase change problems using the fixed grids method: enthalpy, heat capacity, temperature transforming method, and heat source method. Every method has its main distinct feature for the latent heat liberation with advantages and disadvantages. Table 1 summarizes these methods, and highlights the main feature and their advantages and disadvantages. For many reasons including computational efficiency, modeling accuracy and flexibility in selecting solution schemes, the enthalpy method is merited to be an attractive mathematical model over others for simulating phase change problems. In particular, it becomes appealing when the corrective iterative scheme (i.e., a fast and energy conservative approach), or non-iterative scheme (i.e., a quick but conservative approach at low time steps) are implemented. To further exploit these two features for large time steps, a quick but energy conservative approach is envisioned.

4. Models for building enclosures with PCM

A few models have been developed to solve phase change problems on the basis of the general mathematical methods described above. A list of the models for various engineering fields including building applications was reviewed recently by these studies [19,20,83–86]. This section, however, provides a more concentrated and in-depth review on the models that are proposed and used for simulating PCM integrated within building enclosures.

A few innovative and sustainable designs have been proposed by integrating PCM within building construction elements. These designs demand different levels of model complexity to evaluate the thermal performance of such elements. The computational models are classified hereafter as the simplified, intermediate and sophisticated models. Within this context, the simplified models

Table 1
Feature, advantages and disadvantages of mathematical methods used for phase change problems.

Mathematical model for latent heat evolution	Main feature	Advantages	Disadvantages	Possible solution schemes	References
Enthalpy method	Enthalpy accounts for sensible and latent heat	• Fast if proper scheme is selected • Deal with sharp as well as gradual phase change	• Difficult to handle supercooling problems • The temperature at a typical grid point may oscillate with time	Iterative scheme with Non-linear solvers (e.g., Newton's methods) Linearized-Enthalpy: Corrective iterative scheme Quasi-Enthalpy: Non-iterative Temperature correction scheme	[24,55] [22,35] [42]
Heat capacity method	Heat capacity accounts for both sensible and latent heat	• Intuitive since dealing with one dependent variable "Temperature" • Easy to program • Suitable for gradual phase change	• Lack of computational efficiency • Small time step and fine grids are required for accuracy • Difficult in handling cases where the phase-change temperature range is small • Difficult to obtain convergence with this technique, and there is always a chance that the latent heat is underestimated • Not applicable for cases where phase change occurs at fixed temperature	Iterative Scheme (e.g., Gauss–Seidel iterative scheme) if a proper heat capacity approximation is selected	[22,27,29,61,63,64]
Temperature transforming method	Heat capacity and source term are used to account for sensible and latent heat	• Deal with sharp and gradual phase change • Handle large time step and course grids	• Not a common method and therefore not tested to evaluate the pros and cons	Iterative Scheme (e.g., Gauss–Seidel iterative scheme) after linearizing the source term	[43–46,80,81]
Heat source method	Latent heat is treated as a source term	• Intuitive due to separating the latent heat from sensible • Deal with sharp and gradual phase change	• Requires under-relaxation and therefore extra efforts is needed to determine the optimum relaxation factor • Lack of computational efficiency • Problems with round off errors if melting occurs over temperature range	Iterative Scheme (e.g., Gauss–Seidel iterative scheme) after linearizing the source term	[23,38,47,49]

are rough approximations of the physics in the phase change process but offers quick results. The intermediate models are a tradeoff between the speed of the simplified models and the accuracy and flexibility of the sophisticated models. The sophisticated models are created using well validated numerical packages that offer a choice of established and optimized numerical methods. This class offers a high level of accuracy and modeling flexibility but is computationally expensive.

4.1. *The simplified models*

Detailed models for simulating PCM within building enclosures may capture more physics of heat transfer process. However, simplified models are sometimes preferred to provide a quick estimation of PCM's thermal performance. Some simplified models have been developed with this intention [87–91].

A steady-state analytical model for evaluating the benefits of PCM in walls and roofs has been proposed by Kaushik [87]. The model used the heat capacity method to represent the dynamic thermal storage of PCM. The model was utilized to analyze the dynamic thermal performance of a free floating building with PCM embedded in a south wall façade [88]. The result for a typical mild winter day in New-Delhi showed that the wall with PCM outperformed that of an ordinary wall. A rough model utilizing the heat capacity method was developed to characterize the heat transfer process and subsequently estimate the temperature trend in a PCM mixed with gypsum plaster board [89]. The simplified model was able to capture the overall trend of air temperature in the conditioned room. Another simplified physical model using the R–C network method was developed and validated for three wall types: light, medium and heavy with shaped-stabilized phase change material [90]. The model, however, had to use a genetic algorithm to identify the key model parameters: resistances and capacitances of the wall layers to reach an optimal node distribution. When the optimal parameters are identified, the model can be used to simulate the heat transfer process in a wall unit that has a PCM layer. Although the model is intended to be simple, multiple procedures are necessary for practical applications. The model was however implemented to evaluate the energy performance of an office building with shaped-stabilized phase change material embedded in a wall unit [91].

4.2. *The intermediate models*

A variety of intermediate models using, respectively, the enthalpy method, heat capacity method and heat source methods have been developed for one, two and three dimensional cases for building enclosures.

4.2.1. *The enthalpy method*

In the enthalpy method, the enthalpy may be solved by nonlinear solvers with an auxiliary function (e.g., temperature–enthalpy relationship) or implicitly in the governing equation using linearization techniques. A theoretical analysis based on the

enthalpy method was presented in a study evaluating a PCM in a wallboard for solar energy storage [92]. A semi-implicit Crank–Nicolson method was used for numerical discretization, which was subsequently solved using the Newton's method. A more sophisticated two dimensional finite volume heat transfer model based on the enthalpy method was developed and validated to explore the behaviors of phase change materials incorporated into building-integrated photovoltaic (BIPV) system [93,94]. The heat equation is solved with an auxiliary temperature–enthalpy function. The model was utilized to perform an optimization study of commercially available PCM products embedded into cavity-wall systems with different wall-PCM configurations [95]. In addition to simulating heat transfer process, the model has the capability to solve the Navier–Stokes equation (i.e., the momentum and mass equations). The model was expanded later to evaluate a three dimensional heat transfer process with PCM [96]. It was found that the 3D model does not offer additional accuracy when compared to the previously validated 2D model. Another example of a validated finite element 3D numerical model based on the enthalpy method has been suggested to simulate the PCM mixed with common mortars for wall plaster [97].

Using the enthalpy linearization approach, a model was recently presented as an alternative method for a PCM algorithm in ESP-r, a whole building simulation program [60,98]. The MATLAB simulation environment was used to develop a one dimensional numerical model using a corrective iterative scheme proposed by Swaminathan and Voller [35] based on the enthalpy linearization. The customized model in MATLAB uses the finite volume method with a Crank–Nicholson scheme to produce a fair comparison to ESP-r. The model has proven to be accurate and fast when compared to the ESP-r results for a BESTEST Case 600 model configured with PCM.

4.2.2. The heat capacity method

Phase change materials for building applications such as Paraffin melt or freeze over a temperature range compared to pure materials where phase change occurs at fixed temperature [15–17,85]. This property makes the heat capacity method an attractive approach to simulating PCM in building applications. Utilizing MATLAB package, a research group has developed an implicit one dimensional finite difference model for PCM in inner wallboard, ceiling and floor with the heat capacity method [99]. The discretized equation was solved using the Gauss–Seidel iterative method. Although the lab experiments were limited and simulation program was incomplete at that stage, the overall benefits from PCM in wallboard were evident.

A semi-implicit one dimensional finite volume heat transfer model for simulating PCM in a ceiling of a room using the heat capacity method was developed and validated by Pasupathy [100,101]. The model was solved using the tri-diagonal matrix algorithm (TDMA) with very small time step. Although the overall trend of indoor air temperature was captured by the model, the numerical results were not in a good agreement with the experiments due to many limitations of the model. The same model was later used for evaluating the PCM integrated into a roof system [102].

The heat capacity method has also been implemented in a one dimensional numerical model to evaluate shape-stabilized phase change materials embedded with a floor heating system [103]. The specific heat capacity was used to account for the enthalpy of PCM at different temperature regimes. The model gave good agreement results when compared to experimental data. The model was also used for PCM evaluations under different climates and various system configurations [5,104,105]. A variety of modeling applications of PCM embedded in floor system for different purposes using the heat capacity method have been reported in literature [106–108].

PCMs have also been integrated in transparent building envelopes such as glazed windows. An explicit one dimensional finite-difference model based on the heat capacity method was extended to evaluate PCM performance when integrated into a double glazing system [109,110]. The developed model was validated with experimental data and then subsequently utilized to evaluate the impact of PCM on heat loss and gains.

While models developed for building envelope are normally for one dimensional geometry, two and three dimensional heat transfer approaches have also been suggested for modeling PCM using the heat capacity method. In the early 1990s, a numerical code "WALL88" was proposed for modeling two dimensional transient thermal transport and storage of both sensible and latent heat [111]. The model was validated against analytical solution and experimental lab results. The model was found to give an excellent agreement with experimental results only after allowing the PCM to melt over a temperature range rather than at isothermal temperature. A three dimensional finite-difference heat transfer model using the heat capacity method was developed to study the thermal performance of randomly mixed PCM and laminated PCM-wallboard systems [112,113]. Although the numerical model was not validated in these papers, the simulation results were helpful to conclude that laminated PCM-wallboard performs thermally better than the randomly PCM-wallboard. This model was later validated against an experiment and found a maximum of 3% deviation from the average experimental results [114]. The model was further used to evaluate the PCM applications in the drywall in a passive solar building [115]. The results confirmed the conclusions from previous studies for the application of laminated PCM-wallboard. Optimizing the PCM distribution within building envelope is the overall goal of an energy efficient design. The heat capacity method was adopted by an inhouse software "CODYMUR", developed by a team from France, to optimize the use of a PCM wallboard for building energy use [116].

4.2.3. The heat source method

The heat source method is an intuitive approach due to the separation of specific and latent heat. An explicit one dimensional finite-difference heat transfer model for a wall with PCM was developed using the heat source method by Athienitis [117] and validated against a full-scale outdoor test-room with PCM gypsum board at interior side. The model showed a reasonable agreement with experimental results. A heat transfer model of a newly developed hybrid thermal energy storage system (HTESS) using PCM capsules in a wall-unit was developed and validated for managing solar and electric energy [118]. The numerical model uses the heat source method similar to that proposed by Voller [48] where the latent heat evolution is represented by a source term in the governing equation. The fluid fraction is the key to track the latent heat process.

Phase change materials incorporated within floor systems was evaluated using a one dimensional finite volume heat transfer model based on the heat source method [119]. The numerical model was validated with a benchmark analytical solution of Stefan problem explained by Hu [29]. After optimizing the grid and the time resolution, the developed model together with an optimization algorithm was used to perform an optimization analysis on PCM-floor designs. A two dimensional numerical model was developed based on the heat source method to simulate the effect of PCM in the design of a solar passive wall [120]. The model has been verified using benchmark cases documented in literature. The model was later validated using experimental data performed in the Lab and found to be

unsatisfactory due to the limitation of handling the super-cooling effect inherited in the tested PCM [121].

4.3. The sophisticated models

Developing a numerical model in two or three dimensional domain is complicated and difficult to be generalized for different geometries, applications and physics; hence existing simulation packages such as COMSOL (formerly known as FEMLAB) [122], ANSYS-FLUENT [123], HEATING [124] and others are used as convenient design tools. Although, these models offer high level of flexibility, they are not fully explored for heat transfer process with phase change.

One study has used a commercial package FEMLAB (later COMSOL multiphysics) to develop a wall model with phase change materials using the enthalpy method and heat capacity method [125]. COMSOL is a finite element simulation package that allows multi-physics modeling for many engineering applications. Utilizing this package, the created model was validated against experimental results. It was found that both numerical methods give good estimation of latent heat evolution process. However, the heat capacity method found to be more precise with the experimental results when a narrow melting temperature range of 2 °C was selected. COMSOL has also been used to study envelope systems with PCM [126]. The numerical results from COMSOL were successfully compared with another well-established numerical model “WUFI-5”. COMSOL is flexible in modeling multi-physics within irregular and complex geometries. For example, an innovative honeycomb wallboards with PCM have been modeled in a 3D domain using the heat capacity method [127]. The simulation results showed a very good agreement with the experimental results.

A computational fluid dynamics (CFD) simulation package “FLUENT” has been utilized to evaluate a heat source method when using user-defined functions for heating and cooling cycles of PCM rather than using one idealized function to represent both phenomena [128]. The results of a PCM box model utilizing the two functions showed very small error (in root mean square (RMS) values) when compared with a case of using an ideal function for phase change. Another example of using FLUENT is reported for PCM integration into a wall cavity system [129].

Heat Engineering And Transfer In Nine Geometries (HEATING) is a multidimensional, general-purpose heat transfer code that has been extensively validated under ASHRAE project RP-1145 [130]. The code can also be used to model the phase change using the heat capacity method. Ahmad [131] has used the program to study the behaviors of PCM in wallboard of a test cell. The model was validated using experimental test results and found to agree well with experiments. The PCM research program at Oak Ridge National Laboratory (ORNL) has used this program to study the thermal behaviors of PCM in complex two and three geometries in building envelope [132]. Lab tests using a heat flow meter apparatus (HFMA) have been conducted to validate the model in HEATING. HEATING has also been used as a standard benchmark numerical package to validate the finite-difference algorithm used for PCM modeling in EnergyPlus [133].

4.4. Summary

A variety of models for different building enclosures have been developed using various simple, intermediate and sophisticated approaches. Table 2 summarizes the models, application usages, and validations. It is obvious that very few simplified models have

Table 2
Modeling approaches for latent heat evolution in building enclosure.

Complexity level	Latent heat evolution’s approach	Building enclosure case studied	Modeling formulation	Solution strategy	Validation	References
Simplified models						
	Heat capacity method	Wall and roof	Steady-state analytical model			[87,88]
		Wallboard			Experimental	[89]
	Optimum nodes for heat capacity distribution using genetic algorithm	Wall	R-C Network		N/A	[90,91]
Intermediate models						
	Enthalpy method	Wall	FVM: 1D	Newton’s method		[92]
		BIPV	FVM: 2D & 3D	Non-linear solver	Experimental	[93,95,96]
		Wall	FVM: 1D	Iterative corrective scheme	Comparative	[60,98]
	Heat capacity method	Wall	FDM: 1D	G-S	Experimental	[99]
		Ceiling/roof	FVM: 1D	TDMA	Experimental	[100–102]
		Floor	FDM: 1D	G-S	Experimental	[5,103–105]
		Glazed-Windows	FDM: 1D	EM	Experimental	[109,110]
		Wallboard	FDM:2D		Analytical and experimental	[111]
		Wallboard	FDM: 3D		Experimental	[112–115]
	Heat source method	Wall	FDM: 1D	EM	Experimental	[117]
		Wall	FDM: 1D	TDMA	Experimental	[118]
		Wall	FVM: 1D	Iterative scheme	Analytical	[119]
		Wall	FVM: 2D	TDMA	Analytical, comparative and experimental	[120]
Sophisticated numerical packages						
COMSOL	Heat capacity method and heat source method	Wall	FEM: 2D		Experimental	[125]
	Heat capacity method	Wall	FEM		Comparative	[126]
	Heat capacity method	Wall	FEM: 3D		Experimental	[127]
FLUENT	Heat source method	Wall	FVM: 3D	SIMPLE algorithm	Experimental	[128]
	Heat source method	Wall	FVM: 2D		Experimental	[129]
HEATING	Heat capacity method	Wall and roof	FDM: 1D, 2D and 3D	Point-successive over-relaxation iteration	Experimental	[131–133]

FVM: finite volume method, FDM: finite difference method, FEM: finite element method, G–S: Gauss–Seidel iterative method, TDMA: tridiagonal matrix algorithm, EM: explicit time stepping marching, R–C: resistance–capacitance.

been suggested due to the complexity of approximating the heat transfer process associated with phase change. The intermediate models are commonly used but are developed for specific applications and to investigate explicit envelope designs. Hence, they lack flexibility in analyzing complex and advanced design alternatives which becomes norms for selecting optimal or near optimal designs. Sophisticated models offer flexibility in solving complex and multi-physics problems but are not fully explored for modeling PCMs. This is partly due to the computational inefficiency. They additionally demand considerable amount of detailed data inputs, lengthy model setup and validations, and limited access to the source codes.

Generally, all models that adopt the heat capacity or heat source methods must be, however, used with small time steps to attain acceptable accuracy and therefore slow for whole year simulation which is typical for building's thermal performance evaluation. In addition, many existing models ignore inherited characteristics of some PCMs such as hysteresis or subcooling and therefore cannot be used for this particular application.

5. PCM models integrated into whole building simulation programs

Many detailed simulation programs are nowadays available to assist designers, researchers, manufacturing companies to implement new technologies and evaluate innovative ideas that improve the energy and thermal performance of buildings. Detailed simulation tools perform computations on an hourly or sub-hourly bases for accurate considerations of the dynamic interactions between all thermal-based elements associated with comfort and energy consumption, including building envelope, HVAC systems, lighting and control devices [134]. Many building simulation tools are listed at the U.S. Department of Energy (DOE) web directory [135]. The twenty prevalent whole building energy simulation programs that are considered accurate and capable of handling the dynamic behaviors of a building and its systems are reviewed by Crawley et al. [136]. Few whole building simulation programs can handle the thermal performance of building envelope with phase change materials such as EnergyPlus, TRNSYS, ESP-r, and BSim. In addition, some other programs with limited capabilities are available for modeling phase change in buildings. The following paragraphs brief and compare the conditions of these programs.

5.1. EnergyPlus

EnergyPlus uses the Conduction Transfer Functions (CTF) to approximate heat transfer in building envelope. Since the CTF method uses the historical values of heat flux in the computation, Barbour [137] has studied the possibility of using this method in EnergyPlus to approximate the latent heat evolution in building envelope. The study developed multiple sets of CTFs based on the temperature of phase change materials. A switching mechanism was proposed to exchange between these sets during the simulation. The CTF-switching algorithm was found to be within 20% accuracy for a range of conditions typically encountered in buildings.

The capability of modeling PCMs has been facilitated in EnergyPlus program Version 2.0 released in April 2007 by adding a conduction finite difference (CondFD) solution algorithm [138]. The algorithm uses a semi-implicit finite difference scheme based on the heat capacity method with an auxiliary enthalpy–temperature dataset to account for latent heat evolution [139]. Using this dataset, the heat capacity is approximated using a temporal averaging approach similar to that proposed by Morgan [71]. While the previous versions of EnergyPlus had a semi-implicit scheme for modeling PCMs, a fully implicit scheme has been recently added to Version 7 of the program with more numerical flexibility [140]. For both schemes, it is however recommended to use a small time step for accurate results.

Experimental validations have been conducted for this algorithm with mixed feelings of accuracy. Castell, for example [141], found that EnergyPlus simulation results did not show a good agreement with the experiments when phase change materials were implemented in concrete blocks. The study concluded that the simulation results did not reflect the thermal improvement of PCM observed in the test cells. However, the study highlighted that the weather data used in this simulation was not representative of the actual weather data.

An experimental test shed with a commercial PCM product has been used to validate EnergyPlus (Version 5) simulation results under the climatic conditions of Phoenix, Arizona [142]. It was found that the predicted energy consumptions were half during winter and slightly greater for the summer months. In addition, the time shift was observed for a very short time span during the month of April (3 min) and October (9 min).

Under the climatic conditions of Auckland New-Zealand, an experimental study using PCM in gypsum board has been compared to the simulation results of EnergyPlus using both historical weather data and actual measured weather data [143]. Although EnergyPlus model using actual weather data has captured the overall trend of indoor air temperature but failed to accurately predict the actual indoor air temperature from measurements. The study highlighted that due to many parameters including air infiltration, the simulation results might deviate from the actual measurement.

An early successful validation of the CondFD solution algorithm used for PCM modeling has been reported by Zhuang [144] using two envelope systems with PCM: envelope "A" (one layer of PCM: melting temperature at 40 °C) and envelope "B" (two layers of PCM: one melting temperature at 40 °C and another at 33 °C). The study shows that the largest relative difference in indoor temperature is 12.41% and the least is 0.71% between the simulation and testing results in a sequential 36 h period on envelope "*A*" condition. For envelope "*B*" condition, the largest relative difference is 8.33% and the least is 0.33% in a sequential 72 h. It was concluded that the most important factors in reducing the discrepancies between the simulation and the test results are to use proper actual weather data as well as using proper material thermal characteristics. Other successful validations of EnergyPlus algorithm for PCM have been conducted by Campbell [145] and Chan [146] using published experimental data by Kuznik [147]. For both validation studies, the indoor air temperature was found to agree well with the experimental results.

A field test house was used to study the impacts of PCMs in building envelope and consequently used to validate the CondFD algorithm in EnergyPlus [148]. The test house used the cellulose insulation mixed with 20% PCM by mass. The study reported that simulated daily average heat flux through walls was within 9% of the field measurements. In addition, simulation results for temperature distribution through envelope compared fairly well with the experimental data apart from some delayed response compared to the measurement. However, EnergyPlus has given unreasonable results for heat fluxes and temperature distributions in the attic floor of the experimental house.

In addition to the validations above, the EnergyPlus's developer team has performed rigorous validation and verification studies for general heat transfer calculations as well as the CondFD solution algorithm [133,149,150]. These validation studies used analytical benchmark solutions, comparative tests with well-established program "HEATING", and experimental results.

The studies concluded that versions prior Version 7 contains two bugs and subsequently will be fixed in a later version. It is also recommended to follow guidelines and bear in mind limitations in using Version 7:

- The time step should be shorter than 3 min.
- For an accurate hourly thermal performance, 1/3 of the default node space should be used.
- Hysteresis in PCM is not modeled in EnergyPlus and therefore inaccurate results may be produced.

5.2. TRNSYS

TRNSYS is a modular program where components modules “TYPES” are linked together in which output of one type can be an input to another in the model. It has been widely used for modeling building and its complex systems. Due to its modularity, users can either utilize available types in the simulation package or develop new modules and easily integrate to the TRNSYS simulation package. Many features have been introduced in Version 16, including a graphical user interface “Simulation studio” and the possibility to call external programs such as MATLAB, FLUENT and many others [151].

Many models have been proposed in TRNSYS for modeling phase change heat transfer in building envelope but majority are proprietary research modules. Ghoneim for example used a modified type of the thermal storage wall “TYPE36” where the use of PCM has been tested for thermal storage in a wall system [152,153]. The model was based on the enthalpy method and solved using an explicit scheme. Despite the numerical problems encountered when modeling PCM due to the smaller time step required for the stability of the explicit scheme, the model was successfully integrated into TRNSYS and validated against published data for a concrete storage wall. Another explicit numerical scheme using the enthalpy method was developed for modeling the effects of integrating PCM into a solar wall [154,155]. The module “TYPE58” was integrated into TRNSYS to explore the significance of heating outside air for ventilation purposes in the experimental house.

Modeling PCM in TRNSYS is recently provided through “TYPE204” by a team of researchers from Helsinki University of Technology [156]. The model simulates heat transfer through a wall in a three dimensional domain using the Crank–Nicolson scheme with 729 nodes. The model can indeed use a fully implicit or explicit scheme with an appropriate selection of a parameter that switches between different schemes. The model uses the heat capacity to account for latent heat evolution in the wall. Although this type has not been validated in its 3D form due to its poor computational efficiency, Ahmad [157] has converted the 3D model into a 1D module “TYPE101” and validated the modified code. The simulation results were compared to experimental results from two test cells: one without PCM and another with PCM. While the model without PCM works well when compared to the experimental results, the model with PCM overestimates the daily peak indoor temperature in the cell. The authors outlined several reasons for this discrepancy including: (i) evaluation of the energy transmitted through the window, (ii) imprecision in the melting temperature range taken in the heat capacity definition, (iii) values of the convective heat transfer coefficient between wall surfaces and ambient air and (iv) existence of cold bridges. Out of these reasons, it was found that correcting cold bridges by introducing extra term for resistance improved the simulation results significantly when compared to the experimental results.

A study reported a simplified approach of simulating PCM in walls/ceiling and floor in TRNSYS [158]. The approach is to use the existing capability of TRSNYS to simulate a standard active wall in “TYPE56” (i.e., building module in TRNSYS). The key in this approach is a user input of equivalent heat transfer coefficients introduced in each time step of the simulation that characterizes the thermal behaviors of the wall with PCM. The model does not evaluate the real heat transfer behaviors in PCM but accurate enough for modeling PCM thermal behaviors. The model has been validated under laboratory setting conditions.

On the other hand, Schranzhofer et al. [159] have developed a PCM module “TYPE241” where PCM was modeled as an internal layer based on the heat source method. TRNSYS capability was utilized to model other envelope layers using the transfer function method by creating dummy contact zones between the PCM layer and the remaining layers. In this type, the PCM is modeled using external code based on finite different method with other layers modeled through CTF algorithm available internally in TRNSYS “TYPE56”. One advantage of this approach is the short computational time needed for numerical solution but the physics might not be captured well because of assumptions involved in the dummy contact zones. The model however was not validated due to a lack of appropriate experimental data.

Kuznik et al. have recently developed a new model “TYPE260’ in TRNSYS utilizing the heat capacity method [160]. The model is semi-implicit since the physical properties of PCM used in the computations are calculated from previous time step. This type has been validated with two lab tests conducted by authors: one when the outdoor temperature was increased in two steps and the second when it was a sinusoidal behavior. The heating heat capacity curve was used for the numerical modeling. For both validations, the simulation results showed good agreement with the test results.

A newly developed one-dimensional heat transfer model using the heat capacity method was applied to a dividing wall with 16 glass bricks filled with PCM in TRNSYS [161]. The model has been validated and showed fair agreement with experimental results. In addition, a simplified PCM module “TYPE1270” has been recently developed by Thermal Energy System Specialists (TESS) and added to its commercially available individual components [162]. The module simulates PCM as an internal layer within an envelope system. The model is currently limited to materials that melt/freeze at isothermal temperature and with constant specific heat at solid and liquid. In the transition state, the PCM layer temperature is constant and the model tracks the energy absorption and release. The tracking methodology is similar to the heat source method and therefore can be identified as “Quasi-Heat Source Method”.

5.3. ESP-r

ESP-r is a dynamic energy simulation tool of UK, used for modeling thermal, visual and acoustic performance of buildings [163]. With many features suitable to model advance sustainable energy technologies, ESP-r has the capability to model phase change materials using two methods: the effective heat capacity method and the additional heat source method [62,164,165]. ESP-r uses four models for PCM simulation, with one that accounts for sub-cooling, using special materials function. However, it is necessary to use a small time step to obtain accurate results for these two methods. While simulation results using ESP-r have been found in literature, none showed any substantial validations for these two algorithms in ESP-r [166–169].

5.4. BSim

BSim is a dynamic simulation program originated from Denmark that offers an easy user graphical interface [170]. Using

the quasi-steady state in building modeling, the program models phase change using the heat capacity method [171]. The simulation time step has to be small, too, for accurate prediction. Lab test results from literature were used to validate the model on three cases: continuous heating, continuous cooling, and heating but with initial temperature below melting point of PCM. The simulation model captures the overall trend of actual thermal behaviors of PCM but with small deviations.

5.5. Other building simulation programs

Some other building simulation programs have been developed for specific research purposes of modeling phase change materials, such as RADCOOL [172], ESim [173], and CoDyBa [66]. Few have been proposed and developed to simulate simple building configurations, such as PCMExpress [174] or the one using Engineering Equation Solver (EES) [106]. Due to limited

Table 3
Numerical methods for latent heat evolution in building simulation programs.

Building simulation	Module identification	Numerical formulation	Numerical method used for latent heat evolution	Time stepping scheme	Limitations/Constrains	Validation	Reference
EnergyPlus	CondFD	FDM: 1D	Heat capacity method	1. Implicit 2. Semi-implicit	• Time step <3 min • Small grids • Hysteresis in PCM is not modeled • Phase Change at isothermal temperature is not modeled	Analytical, Comparative and Experimental	[133,144–146,148–150]
TRNSYS	Modified “TYPE36”	FDM: 1D	Enthalpy method	Explicit	• Low time step • No access to the code	Limited validation using experimental results for concrete	[152,153]
	“TYPE58”	FDM: 2D	Enthalpy method	Explicit	No access to the code	Experimental	[154]
	“TYPE204”	FDM: 3D	Heat capacity method	Select an appropriate factor for implicit, semi-implicit or explicit	Computationally inefficient	N/A	[156]
	“TYPE101”	FDM: 1D	Heat Capacity Method	Semi-implicit (Crank–Nicolson)	• A correction factor to account for cold bridges has to be used for model accuracy	Experimental	[157]
	TRNSYS “Active Wall”	Equivalent heat transfer coefficients	Variable heat source function mimicking PCM behavior		• Real heat transfer physics in PCM is not modeled	Experimental	[158]
	“TYPE241”	FDM: 1D	Heat source method		No Published data	N/A	[159]
	“TYPE260”	FDM: 1D	Heat capacity method	Implicit	• Thermal properties including heat capacity are based on previous time step (i.e., explicit scheme)	Experimental	[160]
	Modified “TYPE101”	FDM: 1D	Heat capacity method	Implicit	• Developed for Internal partition wall	Experimental	[161]
	“TYPE1270”	Lumped method using heat balance	Quasi-heat source method		• Very simplified model • Internal layer within an envelope • Based on lumped heat balance (not a finite volume), low accuracy • For phase change at fixed temperature	N/A	[162]
ESP-r	SPMCMP53-SPMCMP56	FDM: 1D	Heat capacity and heat source method		• Low time step	N/A	[164,165]
BSim		FVM: 1D	Heat capacity method	Implicit	• Low time step to avoid instability	Experimental	[171]
RADCOOL		FDM: 1D	Heat capacity method	Implicit			[172]
ESim		FDM: 1D	Heat capacity method	Explicit	• Explicit scheme requires low time step to avoid instability	Experimental	[179]

FVM: finite volume method, FDM: finite difference method.

literature available for these programs, only few will be discussed hereafter.

5.5.1. RADCOOL

RADCOOL is a design tool for cooling and heating system developed at the Lawrence Berkeley National Laboratory of the US [175]. The program was created using the simulation problem analysis and research kernel (SPARK) [176]. A one dimensional finite-difference model for a wall with PCM was added to this validated thermal building simulation program [172]. The model was then used to study the capability of a double PCM-wallboard to achieve thermal comfort without using mechanical cooling system under a typical climatic condition of Sunnyvale, California [177].

5.5.2. ESim

ESim was developed at University of Dayton for building energy simulation and can be downloaded from the developer website [178]. The simulation program was expanded and validated to model PCM-wallboards using an explicit finite-difference approach [179]. A list of template files are available for use but with limited capability to model complex buildings and systems.

5.5.3. PCMExpress

PCMExpress is a planning and simulation program for buildings using phase change materials [174], which was developed by a German company, in collaboration with the Fraunhofer Institute for Solar Energy (ISE) in Freiburg and partners from industry [180]. The program simulates a free floating building with a library data for weather and various construction materials including PCM and the flexibility to add new materials. It is an effective tool to evaluate the economic and technical feasibility of PCM usage during an early design stage. The mathematical model of the heat transfer process in PCM is not available. The model has been tested by Castell [141] who found that the simulations deviate significantly from the experiments. As commented by Castell, the discrepancy could be attributed to the lack of accurate infiltration model in the program. The program however has been used to demonstrate the impact of using PCM in residential and commercial buildings [180,181].

5.6. Summary

Whole building simulation programs play an important role for studying the economic and technical feasibility of PCMs. This section reviews the capability of various whole building simulation programs as summarized in Table 3. It is noted that most PCM models integrated into whole building simulation programs are based on the heat capacity method. Hence, it becomes necessary to reduce the typical one hour time step to a very small time step (i.e., in order of minutes) to achieve acceptable level of accuracy. For one year thermal performance evaluation, building simulation programs become computationally inefficient since iterative methods are used in each time step. Additionally, the convergence may not be achieved due to numerical instability especially when PCM enters or leaves the phase change region. With all constraints and limitations above, none of whole building simulation programs are currently implementing efficient mathematical models that are quick, accurate and numerically stable at realistic time step. It becomes important to thoroughly investigate different mathematical models with various numerical approaches for modeling PCMs in whole building simulation programs.

6. Conclusions

Significant heat storage offered by phase change materials is promising and favorable for developing various innovative building energy technologies. To quantify the technical and economic feasibility of PCM-embedded technologies, it requires the development of proper computational models. This study reviews various numerical modeling approaches of phase change problems such as the enthalpy, heat capacity, temperature-transforming and heat source methods. The main features, advantages and disadvantages of each method have been discussed. The discretized form of the heat equation with PCM can either be solved with nonlinear solvers such as Newton's methods or via linearizing the nonlinear term and using linear solvers such as iterative methods. For both approaches, the numerical solutions are computationally inefficient or difficult to reach convergence. Therefore, fast numerical schemes are suggested such as the quasi enthalpy non-iterative scheme or the enthalpy conservative iterative scheme.

Using these general mathematical methods, different computational models have been developed to simulate PCMs in building enclosures. Based on the level of complexity, models are classified into three categories: simple, intermediate and sophisticated models. Majority of these models have been validated using analytical solutions, comparative testing using validated numerical models, and/or experimental results.

While many models are used to study the heat transfer in an enclosure unit, a few models have been integrated into whole building simulation programs. A variety of models are available and some are available with no cost to users such as EnergyPlus, ''TYPE204'' in TRNSYS or ESP-r. These particular models, however, have limitations on modeling PCM including the time and spatial resolutions, inability to model hysteresis, lack of validations of some models, and poor computational efficiency. These modeling challenges add complexity to the already existing uncertainties in experimental results of PCM's thermal behaviors. Therefore, further research is needed to quantitatively explore the prediction performance of different models including their limitations on accuracy, parameters sensitivity, speed, and stability for modeling PCM envelopes under different climatic and operating conditions.

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